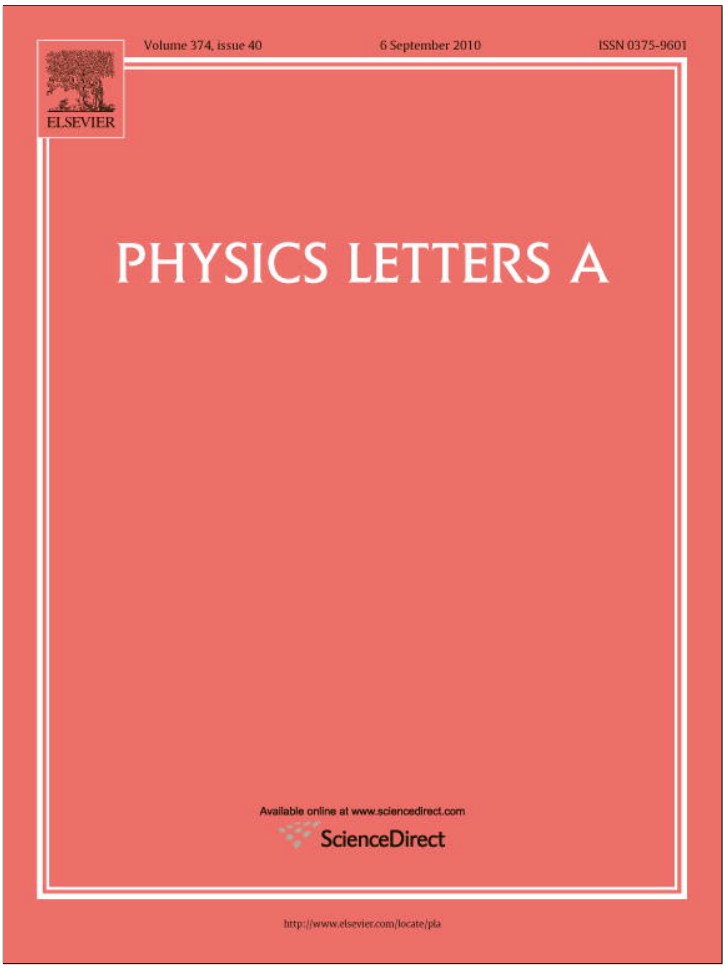

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Electron self-trapping and self-focusing in periodic chains with a finite nonlinear response time

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ABSTRACT

In this work we investigate the one-electron wave-packet dynamics in finite closed chains with relaxational nonlinearity. We found that, besides exhibiting the well-known self-trapping regime at strong coupling, the non-instantaneous character of the nonlinearity favors the self-focusing of the wave-packet at intermediate coupling strengths.

1. Introduction

In transport phenomena, an important problem is the role of electron–phonon interactions in electronic transport, usually analyzed with the help of the discrete nonlinear Schrödinger equation (DNLSE) [1–5]. The interactions of the lattice on moving electrons is the responsible for the self-trapping [3] phenomena, which occurs when the probability of finding the particle at the initial site remains finite. Self-trapping takes place when the nonlinearity parameter is much larger than the bandwidth and, for low-dimensional systems, the effect of nonlinearity is preponderant over disorder [6–10]. By considering a discrete nonlinear Schrödinger and quartic Klein–Gordon equations with disorder, the spreading of an initially localized wave packet was studied in detail [6]. It was proved that the second moment and the participation number of a wave packet do not diverge simultaneously [6]. In Ref. [7], by considering the discrete nonlinear Schrödinger, it was numerically demonstrated that the Anderson localization is destroyed and a sub diffusive dynamics takes place above a certain critical nonlinearity strength. Moreover, analytical and numerical calculations for a reduced Fermi–Pasta–Ulam chain demonstrated that energy localization does not require more than one conserved quantity [9].

From the experimental point of view, the interplay between disorder and nonlinearity was investigated in Ref. [10]. The evolution of linear and nonlinear waves in coupled optical waveguides patterned on an AlGaAs substrate were directly measured. Nonlinear perturbations enhance localization of linear waves while induce delocalization of the nonlinear ones [10]. The nonlinearity and the self-trapping phenomena are important in several other systems. For example, Ref. [11] reported the first experimental observation of nonlinear self-trapping of Bose-condensed atoms in a one-dimensional waveguide with a superimposed deep periodic potential. By controlling the degree of nonlinearity the system's state changes from a diffusive regime, characterized by an expansion of the condensate, to the self-trapping regime, where the initial expansion stops and the width remains finite. The self-trapping dynamics was compared with numerical solutions of the nonlinear Gross–Pitaevskii equation [11]. In Ref. [12] the self-trapping phenomenon of Bose–Einstein condensates (BEC) in optical lattices was studied by numerically solving the Gross–Pitaevskii equation, showing a good agreement with the experimentally observed self-trapping phenomenon [11]. In addition, it was shown that the self-trapping in optical lattices is only temporary and that it has a finite lifetime [12].

The existence of self-trapping, stable, moving solitons and breathers of Fermi wave packets in optical lattices along the (BEC)–Bardeen–Cooper–Schrieffer (BCS) crossover was recently predicted, both analytically and numerically [13]. The stable moving soliton and breather solutions of Fermi wave packets exist along the BEC–BCS crossover for low-dimensional systems. However, for three-dimensional geometries, the stable moving soliton and breather solutions can exist only in the BCS state [13]. Another interesting problem is the self-focusing [14,15]. In this case, the wave function initially spreads over the lattice but ultimately concentrates in a finite region. Recently, it was demonstrated the explicit forms

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for the rational self-focusing solutions in the discrete nonlinear Schrödinger equation [14]. The study of rational self-focusing solutions are of fundamental importance to understand the emergence of rogue waves in the ocean, as well as it can bring new insights that may be used to create and control useful rogue waves in optical fibers [15].

Usually, the nonlinearity that results from an electron–phonon coupling is obtained after considering the adiabatic approximation [16,17]. Within this approach, the nonlinear term couples instantaneously the wave-function with the local electronic density. Non-adiabatic nonlinear models have been studied in a series of works [18–20]. It has been shown that new phenomena arises associated with the relaxation of the nonlinearity, such as the emergence of a stationary self-trapping regime and the coexistence of stationary and dynamical transitions for certain degrees of nonlinearity and relaxation time in dimer-like systems. Recently, the influence of the nonlinear response time on the electronic transport in linear chains was investigated [21]. In the proposed model, a delayed nonlinear term couples the electronic wave-function at time t with the electron density at time $t-\tau$. While a long response time naturally reduces the tendency of self-trapping, it was shown that a short response time counter-intuitively reduces the critical nonlinear strength above which self-trapping takes place. A dynamical transition was also reported on which the wave-fronts start to widen after an initial regime of soliton-like propagation.

Here, we further investigate the influence of the non-instantaneous character of the nonlinear coupling on the electronic transport along linear chains. By considering that the nonlinear coupling obeys a Debye-like relaxation law, as introduced in Ref. [18], we will solve the time-dependent nonlinear Schrödinger equation to follow the time-evolution of an initially localized wave packet in finite chains with periodic boundary conditions. We will show that the Debye relaxation nature of the nonlinearity is responsible for the emergence of new phenomena such as the significant reduction of the asymptotically delocalized regime and a complex wave packet self-focusing regime.

The Letter is organized as follows. Section 2 presents our model and formalism. Section 3 presents the numerical results and discussions and Section 4 concludes.

2. Model and formalism

Let us consider a delayed DNLSE

$$i\frac{dc_n(t)}{dt} = V\left(c_{n+1}(t)+c_{n-1}(t)\right)+X_n c_n(t),$$
$$\frac{dX_n(t)}{dt} = \frac{1}{\tau}\left(-X_n(t)-\chi\left|c_n(t)\right|^2\right), \quad n=1,\ldots,N. \tag{1}$$

Here N is the size of the linear chain and we consider periodic boundary conditions. $c_n(t)$ denotes the time dependent wavefunction amplitude at site n ($|\psi\rangle=\sum_{n=1}^{N} c_n|n\rangle$). The second equation describes the dynamics of the lattice vibrations. The nonlinear parameter χ is proportional to the local electron–phonon coupling under an adiabatic approximation [22], which occurs when $X_n(t)=-\chi|c_n(t)|^2$ and/or $\tau=0$. The delayed DNLSE model used here (Eq. (1)) was derived following the assumptions put forward in Ref. [18]. The model starts by considering a set of $2N$ coupled equations. Half of them corresponds to the wave packet dynamics of the moving quantum particle. The other half corresponds to the motion equation of Einstein-like site oscillators. X_n is the displacement of the oscillator at site n, which has a typical frequency ω and is damped at a rate α. By assuming the oscillators to reach their equilibrium position much faster than the typical time scale for the quantum particle evolution, the time derivative of X_n can be disregarded, thus resulting in the well-known adiabatic DNLSE with a nonlinear contribution to the on-site energy given by $-\chi|c_n(t)|^2$ [18]. In the strong damping regime the set of coupled equations reduces to the delayed DNLSE (Eq. (1)) with $\tau=\omega^2/\alpha$. The non-adiabatic character is incorporating by explicitly solving the relaxation equation considering a finite response time $\tau\neq 0$.

In what follows, we consider the hopping integral between nearest-neighbor sites $V=1$ and the on-site energy is assumed zero. To analyze the wave propagation, we solve (1) using the eighth-order Runge–Kutta method to obtain the temporal evolution of an initially localized wave packet:

$$\begin{cases} n=1 \rightarrow c_n(0)=1, \\ n\neq 1 \rightarrow c_n(0)=0. \end{cases} \tag{2}$$

In order to follow the time evolution of the wave packet, we will compute some representative dynamical quantities that bring information regarding the extension of the wave packet and it's actual location. One of these quantities is the return probability, defined as [23–27]

$$R(t)\equiv\left|c_1(t)\right|^2. \tag{3}$$

Usually, the electron escapes from its initial position when the amplitude $c_1(t)$, and consequently the return probability, vanishes as t evolves. Conversely, the amplitude remains finite for a wave packet localized around its initial position. However, the return probability does bring enough information about the wave packet distribution along the system. In addition, we rely on the participation function to analyze the wave packet extension

$$P(t)=\frac{1}{\sum_{n=1}^{N}|c_n(t)|^4}. \tag{4}$$

The participation function $P(t)$ varies from 1 to N [23–30]. This function gives information about the number of sites that are visited during the time evolution of the wave packet over the underlying lattice.

We also computed a third quantity in order to explore the possibility of the wave packet to become localized in the opposite side of the closed chain. The occupancy probability of the opposite site $O(t)$, calculated at the $(1+N/2)$-th site is given by:

$$O(t)=\left|c_{1+N/2}(t)\right|^2. \tag{5}$$

In the following results, we will show that there are particular cases on which the wave packet focus in the opposite side of the chain after spreading over the lattice.

3. Results and discussion

In order to obtain the quantities $R(t)$, $O(t)$ and $P(t)$, a eighth-order Runge–Kutta method with $\delta t=0.005$ is employed to integrate the delayed DNLSE. The norm conservation was checked at every time step to ensure the numerical convergence.

In Fig. 1, we show the return probability and the participation number versus χ at $t\rightarrow\infty$ in the case of instantaneous nonlinear response (adiabatic regime) for two values of N. The data show the usual behavior exhibited by the DNLSE [2,3]. For $\chi>3.5$ the return probability $R(t)$ is finite and $P(t)/N$ vanishes, suggesting a localized state near the site initially occupied by the wave packet. This is the self-trapping behavior with the electron remaining localized due the electron–phonon interaction. For $\chi<3.5$ the return probability approaches zero and the normalized participation function $P(t)/N$ is finite. Therefore the asymptotic wavefunction in this regime corresponds to an extended state with the wavefunction spreading through the entire lattice.

In Fig. 2, we start to analyze the effect of the nonlinearity relaxation time by reporting $R(t)$ and $O(t)$ versus χ at $t\rightarrow\infty$. All

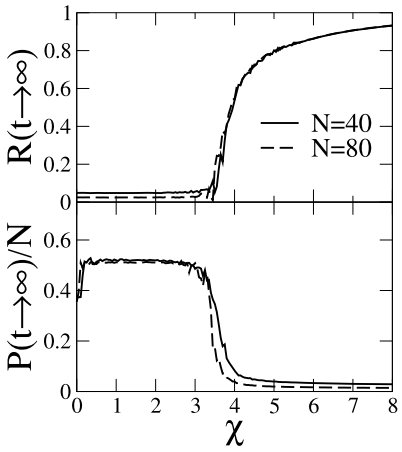

Fig. 1. Return probability $R(t \to \infty)$ and normalized participation number $P(t \to \infty)/N$ versus χ for the case of instantaneous nonlinear response. For $\chi > 3.5$ the return probability $R(t \to \infty)$ is finite and $P(t \to \infty)/N$ vanishes, suggesting a localized (self-trapped) state. For $\chi < 3.5$ the return probability approaches zero proportional to $1/N$ and the normalized participation function is finite, the typical behavior of delocalized wave packets.

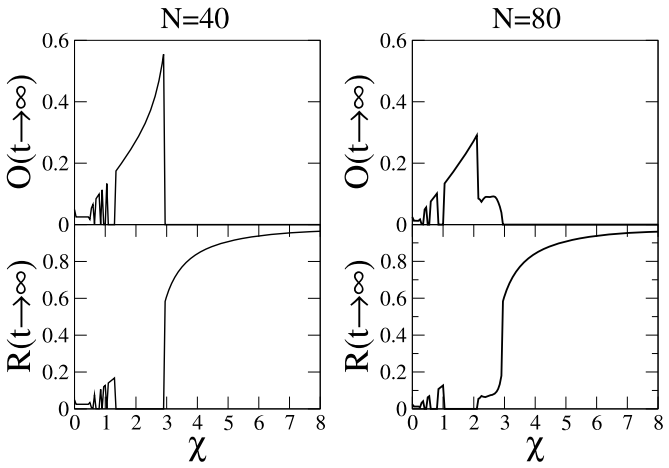

Fig. 2. $R(t \to \infty)$ and $O(t \to \infty)$ versus χ for the case of a finite nonlinear response time $\tau = 1$. Two representative chain sizes are illustrated. For large χ, we observe self-trapping as in the case of instantaneously responding media. Notice that the regime of delocalized asymptotic wave packets is restricted to very small nonlinear strengths. For a chain with $N = 40$ sites, the asymptotic wave packet in the regime of intermediate nonlinearities becomes concentrated either around the initial site or around the opposite site. The actual location of the asymptotic wave packet depends on the system size. For a chain with $N = 80$ sites, it can even become simultaneously distributed around both regions.

results will be shown for the particular case of a relaxation time $\tau = 1$. For $\chi > 3$ the return probability is always finite and the occupancy probability of the opposite site vanishes. This is the typical behavior attained in the large χ regime of instantaneously responding media corresponding to the wave packet self-trapping. For smaller values of χ the wave packet shows an irregular sequence of localization around either the initial site or the opposite site. Actually, there is also a small window of nonlinear strengths on which the wave packet splits into two packets distributed simultaneously on two regions. Such splitting is not observed in small chains. Further, the sequence of transitions depends on the chain size. For small nonlinear strengths, the return and opposite probabilities scale as $1/N$, thus indicating that the wave packet spreads over the entire chain. However, this regime of extended asymptotic wave packet is significantly reduced as compared to the one taking place in instantaneously responding media. Also, this critical nonlinear strength separating the regime of extend and

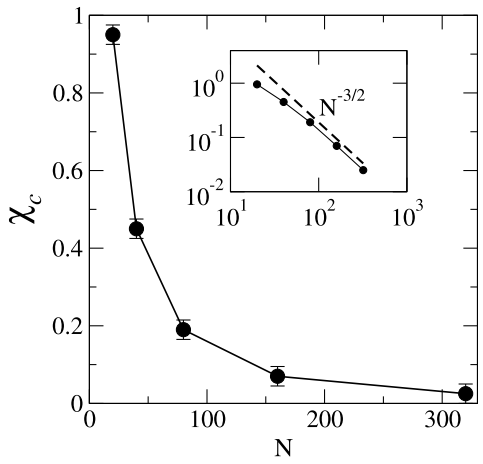

Fig. 3. Critical nonlinearity χ_c versus N. Below χ_c the asymptotic wave packet remains extended over the entire lattice. The phase of extended states is suppressed as the chain size increases. The inset shows that, for large chain sizes, $\chi_c \propto 1/N^{3/2}$.

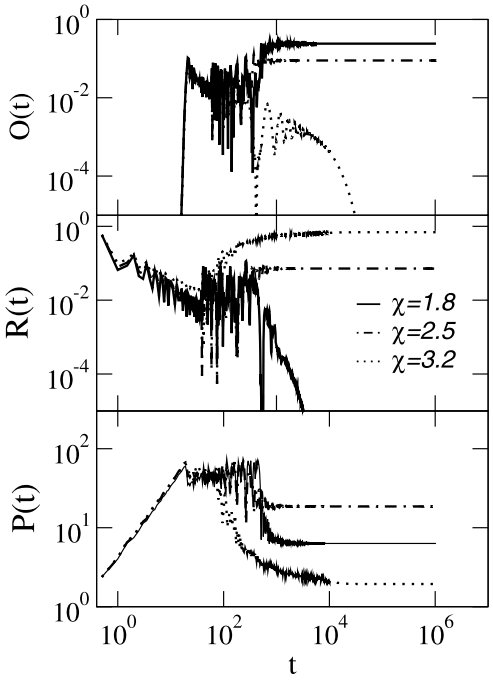

Fig. 4. $R(t)$, $O(t)$ and $P(t)$ versus time for three representative values of χ, considering a chain with $N = 80$ sites and a nonlinear response time $\tau = 1$. All cases show that the wave packet initially spreads (growing participation function) until reaching an intermediate plateau during which the participation function remains of the order of the chain size (delocalized wave packet). A dynamical transition takes place and the participation function decreases until reaching a final asymptotic value (self-focusing). The illustrated cases correspond to self-focusing around the opposite site ($\chi = 1.8$: finite $O(t \to \infty)$ and vanishing $R(t \to \infty)$), simultaneously around both regions ($\chi = 2.5$: both $O(t \to \infty)$ and $R(t \to \infty)$ finite) and around the initial site ($\chi = 3.2$: finite $R(t \to \infty)$ and vanishing $O(t \to \infty)$).

localized asymptotic wave packets decreases as the chain size is increased. The dependence of χ_c on the chain size is depicted in Fig. 3.

In order to develop a deeper understanding of the wave packet dynamics in the regime of intermediate nonlinear strengths, we plot in Fig. 4 the time evolution of the return and opposite probabilities, as well as the time evolution of the normalized participation function in a chain with $N = 80$ sites. Three representative values for the nonlinear strength are illustrated, corresponding to asymptotic wave packets located around the opposite site ($\chi = 1.8$), around the initial site ($\chi = 3.2$) and splitted on both

regions ($\chi = 2.5$). In all cases there is an initial transient during which the initially localized wave packet spreads over the lattice, signaled by an increasing participation function. This initial transient lasts until the wave packet become spread over the entire lattice. After this initial transient, there is a plateau interval in the participation function during which the wave packet remains delocalized over the lattice with similar occupancy probabilities on the initial and opposite sites. The duration of this intermediate dynamical regime depends on the nonlinear strength. After this plateau, the wave packet starts to focus on a finite chain segment. This self-focusing phenomena is strongly enhanced by the relaxation of the nonlinearity. In instantaneously responding media, it only takes place in a narrow interval of nonlinear strengths near the self-trapping transition. Further, self-focusing leads to the localization of the wave packet in distinct regions of the chain, depending on the precise value of the nonlinear coupling. In the illustrated case of a chain with $N = 80$ sites, the wave packet can even self-focuses simultaneously in the regions around the initial and opposite sites. We have observed that new windows with self-focusing on three or more regions appear as the chain size is further increased. Finally, in the regime of strong nonlinear strengths ($\chi > 4$), the intermediate plateau corresponding to fully delocalized wave packets is suppressed. The wave packet remains trapped around its initial position, although it can eventually expand over a large portion of the chain before finally contracting to its final profile.

4. Summary and concluding remarks

In summary, we analyzed the one-electron wave packet dynamics in closed chains with a relaxational nonlinearity originated from an intrinsic electron–phonon coupling. Going beyond the usual adiabatic approach, the response time of the nonlinearity τ is considered explicitly through a Debye relaxation process. We numerically solved a time dependent Schrödinger equation for the electronic wave packet amplitudes simultaneously with a Debye relaxation of the electron–phonon coupling. We found that the wave packet dynamics is strongly sensitive to the non-instantaneous character of the nonlinearity. In contrast with the behavior derived from the adiabatic approach, which provides a wide stability region of asymptotically delocalized wave packets, the introduction of a finite response time makes the delocalized state unstable at finite nonlinear strengths larger than $\chi_c = \mathcal{O}(1/N^{3/2})$. It is interesting to note that a modulational instability analysis in nonlinear optical waveguides also showed that CW waves become unstable with respect to harmonic perturbations in the whole frequency spectrum when the non-instantaneous character of the nonlinear optical response is taken into account [31]. Our present results show that after spreading over the chain, the one-electron wave packet self-focuses on a finite segment. The position of the focused wave packet depicts an irregular dependence on the nonlinear coupling, alternating from the initial site, the opposite site or more complex mixed focused states. Self-trapping still takes place at large nonlinear couplings on which the wave packet remains concentrated around its initial position without an intermediate delocalized dynamical regime. It would be valuable to develop a linear stability analysis to analytically determine the dependence of the critical nonlinear strength delimiting the transition from delocalized and self-focused stationary wave packets. Also, the precise location of the transition from the self-focusing to the self-trapping regime, as well as those corresponding to the dynamical transitions leading to distinct focused states, requires a careful finite-size scaling analysis of the intermediate dynamical regime in order to reveal the mechanism leading to the instability of delocalized wave packets. These aspects evidence the complexity of the electron wave packet dynamics in media with a finite nonlinear response time. We hope the phenomenology here reported will stimulate further studies along these lines, thus covering an important, although still not properly addressed, aspect of the electronic transport in nonlinear systems.

Acknowledgements

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